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Field theoretical approach to the study of theta dependence in Yang-Mills theories on the lattice

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Abstract

We discuss the extension of the field theoretical approach, already used in the lattice determination of the topological susceptibility, to the computation of further terms in the expansion of the ground state energy $F(\theta)$ around $\theta = 0$ in $SU(N)$ Yang-Mills theories. In particular we determine the fourth order term in the expansion for $SU(3)$ pure gauge theory and compare our results with previous cooling determinations. In the last part of the paper we make some considerations about the nature of the ultraviolet fluctuations responsible for the renormalization of the lattice topological charge correlation functions; in particular we propose and test an ansatz which leads to improved estimates of the fourth and higher order terms in the expansion of $F(\theta)$.

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1. Introduction

The dependence of $SU(N)$ Yang–Mills theories on the θ angle is the subject of ongoing theoretical debate. The dependence can be expressed in terms of the free energy density $F(\theta)$ which, in the Euclidean theory, is defined as follows:

$$\exp[-VF(\theta)] \equiv Z(\theta) = \int [dA]\, e^{-\int d^4x \mathcal{L}(x)}\, e^{i\theta Q} \,, \tag{1.1}$$

where V is the four dimensional volume, $\mathcal{L}(x) = \frac{1}{4}F^a_{\mu\nu}(x)F^a_{\mu\nu}(x)$ is the usual Yang-Mills langrangian and $Q = \int \mathrm{d}^4x\; q(x)$ is the topological charge, with the topological charge density $q(x)$ defined as

$$q(x) = \frac{g^2}{64\pi^2}\epsilon_{\mu\nu\rho\sigma}F^a_{\mu\nu}(x)F^a_{\rho\sigma}(x) = \partial_\mu K_\mu(x) \,, \tag{1.2}$$

where $K_\mu(x)$ is the Chern current

$$K_\mu = \frac{g^2}{16\pi^2}\epsilon_{\mu\nu\rho\sigma}A^a_\nu\left(\partial_\rho A^a_\sigma - \frac{1}{3}gf^{abc}A^b_\rho A^c_\sigma\right) \,. \tag{1.3}$$

The coefficients of the Taylor expansion of $F(\theta)$ around $\theta = 0$,

$$F(\theta) = \sum_{k=0}^{\infty}\frac{1}{k!}F^{(k)}(0)\theta^k \,, \tag{1.4}$$

are related to the connected expectation values of the topological charge distribution,

$$F^{(k)}(0) \equiv \frac{d^k}{d\theta^k}F(\theta)|_{\theta=0} = -i^k\frac{\langle Q^k\rangle_c}{V} \,, \tag{1.5}$$

where $\langle\cdot\rangle_c$ is a short notation meaning the connected expectation value taken at $\theta = 0$.

$F(\theta)$ is a non-trivial function, indeed the topological susceptibility, $\chi = \langle Q^2\rangle_c/V$, is expected to be different from zero, to the leading order in $1/N$, to solve the so–called $U(1)$ problem [1, 2]. In Refs. [3, 4] it has been argued that, in the large N limit, $F(\theta)$ is a multibranched function of θ, and in particular

$$F(\theta) = F(0) + \frac{\chi}{2}\min_k(\theta + 2\pi k)^2 + O(1/N) \,. \tag{1.6}$$

Therefore, for sufficiently small values of θ ($\theta < \pi$), $F(\theta)$ is expected to have an almost quadratic dependence on θ, with $O(\theta^4)$ corrections suppressed by powers of $1/N$.

Numerical Monte Carlo simulations on the lattice are a natural tool to obtain information from first principles about the dependence of $F(\theta)$ around $\theta = 0$. While direct numerical simulations of the theory at $\theta \neq 0$ are not feasible because of the complex nature of the action, the Taylor expansion of $F(\theta)$ around $\theta = 0$ can be computed, in principle up to any given order, by measuring the connected expectation values of the topological charge over the ensemble of configurations at $\theta = 0$, as explicited in Eqs. (1.4) and (1.5). The topological susceptibility has been already extensively studied on the lattice (see Refs. [5, 6] for recent reviews) and further terms in the expansion have been recently measured [7].

The lattice study of quantities related to topology requires care. The problem is usually related to the fact that the topology of gauge configurations on a discretized space-time is, strictly speaking, always trivial, and that the usual lattice definition, given in terms of gauge fields as a naïve discretization of the continuum topological charge, does not have the continuum integer valued spectrum: as a good alternative the fermionic definition, which is directly related to the index theorem, or the definition based on the so-called cooling method, are used.

In fact, the topological charge operator and its correlation functions can be defined on the lattice with the same rigour as for any other operator of the theory: as for any other physical quantity, one has to pay attention when removing the ultraviolet (UV) regulator, i.e. when going to the continuum limit, since the appropriate renormalizations have to be performed. In the cooling method the UV lattice fluctuations, which are responsible for the renormalizations, are removed by a process of local minimization of the action. However it is also possible to compute the renormalizations and perform the appropriate subtractions. This program, usually known as the "field theoretical method", has been already widely discussed and developed, together with a method for the numerical non-perturbative determination of the renormalization constants, usually known as the "heating method", in the context of the lattice determination of the topological susceptibility [8, 9, 10, 11, 12, 13, 14, 15, 16].

The aim of the present paper is that of discussing the extension of the field theoretical method (and of the heating method used to compute the renormalizations) to the case of higher order correlation functions of the topological charge, in order to study the θ dependence of the theory. In Section 2, after a review of the field theoretical method, as used for the computation of the topological susceptibility, we will discuss its application to the case of higher order correlations and develop a suitable extension of the heating method. In Section 3 the case of $SU(3)$ pure gauge theory will be used as a testground for the method developed in Section 2, and we will determine the fourth order contribution to $F(\theta)$ and compare our results with those obtained by the cooling technique [7]. In Section 4 we will state and test an ansatz about the nature of the UV lattice fluctuations responsible for the renormalizations, which will allow us to simplify the computation of the connected correlation functions and to obtain more precise determinations of the fourth order contribution to $F(\theta)$. Finally, in Section 5, we will give our conclusions.

2. Topological charge correlation functions on the lattice

In this Section we will discuss how the various moments of the lattice topological charge distribution renormalize with respect to the continuum ones, and how the corresponding renormalizations can be computed numerically. In order to make the discussion clearer, we will first review the case of the second moment, i.e. the topological susceptibility.

2.1. Renormalization of the topological susceptibility

On the lattice it is possible to define a discretized gauge invariant topological charge density operator $q_L(x)$, and a related topological charge $Q_L = \sum_x q_L(x)$ (with the sum extended over all lattice points), with the only requirement that, in the formal (naïve) continuum limit,

$$q_L(x) \stackrel{a\to 0}{\sim} a^4 q(x) + O(a^6) \ , \tag{2.1}$$

where a is the lattice spacing. A possible definition is

$$q_L(x) = \frac{-1}{2^9 \pi^2} \sum_{\mu\nu\rho\sigma=\pm 1}^{\pm 4} \tilde{\epsilon}_{\mu\nu\rho\sigma} \mathrm{Tr} \left(\Pi_{\mu\nu}(x) \Pi_{\rho\sigma}(x) \right) \ , \tag{2.2}$$

where $\Pi_{\mu\nu}(x)$ is the usual plaquette operator in the $\mu\nu$ plane, $\tilde{\epsilon}_{\mu\nu\rho\sigma}$ is the standard Levi–Civita tensor for positive directions and is otherwise defined by the rule $\tilde{\epsilon}_{\mu\nu\rho\sigma} = -\tilde{\epsilon}_{(-\mu)\nu\rho\sigma}$.

A proper renormalization must be performed when going towards the continuum limit, like for any other regularized operator. In spite of the formal limit in Eq. (2.1), the discretized topological charge density renormalizes multiplicatively [8]:

$$q_L(x) = Z(\beta) a^4(\beta) q(x) + O(a^6) \ , \tag{2.3}$$

with a multiplicative renormalization constant $Z(\beta)$ which is a finite function of the bare coupling $\beta = 2N/g_0^2$, approaching 1 as $\beta \to \infty$.

When defining the topological susceptibility, further renormalizations can appear. Indeed, already the continuum definition,

$$\chi \equiv \frac{\langle Q^2 \rangle}{V} = \int \mathrm{d}^4 x \ \langle q(x) q(0) \rangle \ , \tag{2.4}$$

involves the product of two operators $q(x)$ at the same point: this contact term is divergent and not well defined, so that an appropriate prescription must be assigned. It can be shown [17, 18] that the correct prescription, corresponding to the quantity which appears in the Taylor expansion of $F(\theta)$, is the one in which the derivative appearing in the definition of $q(x)$, Eq. (1.2), is taken out of the vacuum expectation value:

$$\chi = \frac{1}{V} \int \mathrm{d}^4 x \mathrm{d}^4 y \ \partial_\mu^x \partial_\nu^y \langle K_\mu(x) K_\nu(y) \rangle \ . \tag{2.5}$$

The lattice definition of the topological susceptibility

$$\chi_L = \sum_x \langle q_L(x) q_L(0) \rangle \tag{2.6}$$

is in general not guaranteed to meet the correct continuum prescription for the contact term, and this leads to the appearance of additive renormalizations:

$$\chi_L = Z(\beta)^2 a^4(\beta) \chi + M(\beta) \ , \tag{2.7}$$

where $M(\beta)$ describes generically the mixing with all local scalar operators appearing in the operator product expansion (OPE) of $q_L(x) q_L(0)$ as $x \sim 0$ in Eq. (2.6), including in particular the action density and the identity operator.

The idea behind the numerical technique, known as the heating method, used to compute the two renormalizations $Z(\beta)$ and $M(\beta)$, is that the UV fluctuations in $q_L(x)$, which are responsible for renormalizations, are decoupled from the background topological signal so that, starting from a semiclassical configuration of fixed and well known topological content, it is possible, by applying a few thermalization steps (i.e. Monte Carlo updating steps at the corresponding value of β), to thermalize the UV fluctuations without altering the background topological content. This is certainly true for high enough β, i.e. approaching the continuum limit, and in practice it turns out to be true in a range of the β values usually chosen in Monte Carlo simulations of Yang-Mills theory, being also favoured by the fact that topological modes have very large autocorrelation times, as compared to any other non-topological mode.

It is thus possible to create samples of configurations which have a fixed topological content, Q, and the UV fluctuations thermalized: various measurements of topological quantities on these samples can give information about the renormalizations. For example the expectation value of Q_L gives

$$\langle Q_L \rangle = Z(\beta)\, Q \tag{2.8}$$

from which the value of $Z(\beta)$ can be inferred, while the expectation value of $\langle Q_L^2 \rangle$ gives

$$\langle Q_L^2 \rangle = Z(\beta)\, Q^2 + V\ M(\beta)\ , \tag{2.9}$$

where by V we intend, from now on, the four dimensional volume measured in adimensional lattice units.

To check that UV fluctuations have been thermalized, one looks for plateaux in quantities like $\langle Q_L \rangle$ or $\langle Q_L^2 \rangle$ as a function of the heating steps performed: only configurations obtained after the plateau has been reached are included in the sample. Special care has to be paid to verify that during the heating procedure the background topological charge is left unchanged: this is usually done by performing a few cooling steps on a copy of the heated configuration and configurations where the background topological content has changed are discarded from the sample [13]. Further details about the procedure and about the estimate of the systematic errors involved can be found in Ref. [14].

A sample with $Q \simeq 1$ can be used to measure Z and a sample with $Q = 0$ (usually thermalized around the zero field configuration) can be used to determine M. Cross-checks can then be performed, using samples obtained starting from various semiclassical configurations with the same or different values of Q, to test the validity of the method.

Once the renormalizations have been computed and the expectation value χ_L over the equilibrium ensemble has been measured, the physical topological susceptibility χ can be extracted, using Eq. (2.7), as

$$\chi = \frac{\chi_L - M(\beta)}{a^4(\beta) Z(\beta)^2} \tag{2.10}$$

If large renormalization effects are present, i.e. if $Z \ll 1$ and if M brings a good fraction of the whole signal in χ_L, the final determination of χ, obtained via Eq. (2.10), can be affected by large error bars. However one can exploit the fact that Z and M both depend on the lattice discretization $q_L(x)$ and that infinitely many operators $q_L(x)$ can be defined all having the same naïve continuum limit, to choose improved operators for which the renormalization effects are reduced, thus leading to improved estimates of χ. This is the idea behind the definition of smeared operators [19]

$$q_L^{(i)}(x) = \frac{-1}{2^9\pi^2} \sum_{\mu\nu\rho\sigma=\pm1}^{\pm4} \tilde{\epsilon}_{\mu\nu\rho\sigma} \mathrm{Tr}\left(\Pi_{\mu\nu}^{(i)}(x)\Pi_{\rho\sigma}^{(i)}(x)\right) \ , \tag{2.11}$$

where $\Pi_{\mu\nu}^{(i)}(x)$ is the plaquette operator constructed with i–times smeared links $U_\mu^{(i)}(x)$, which are defined as

$$\begin{aligned} U_\mu^{(0)}(x) &= U_\mu(x) \ , \\ \overline{U}_\mu^{(i)}(x) &= (1-c)U_\mu^{(i-1)}(x) + \frac{c}{6}\sum_{\substack{\alpha=\pm1 \\ |\alpha|\neq\mu}}^{\pm4} U_\alpha^{(i-1)}(x)U_\mu^{(i-1)}(x+\hat{\alpha})U_\alpha^{(i-1)}(x+\hat{\mu})^\dagger, \\ U_\mu^{(i)}(x) &= \frac{\overline{U}_\mu^{(i)}(x)}{\left(\frac{1}{3}\mathrm{Tr}\overline{U}_\mu^{(i)}(x)^\dagger\overline{U}_\mu^{(i)}(x)\right)^{1/2}} \ , \end{aligned} \tag{2.12}$$

where c is a free parameter which can be tuned to optimize the improvement. These operators have been successfully used, up to the second smearing level, to determine χ at zero and finite temperature both in $SU(2)$ [15] (with $c = 0.85$) and $SU(3)$ [14] (with $c = 0.9$) pure gauge theory. We will make reference to them later in this paper, when computing the higher order correlation functions of the topological charge.

2.2. Renormalization of higher order correlation functions

In order to compute the higher order connected moments of the topological charge distribution, $\langle Q^n\rangle_c$, needed for the Taylor expansion of $F(\theta)$, it is necessary to first compute the disconnected correlation functions $\langle Q^n\rangle$. We will consider in particular the case $n = 4$, for which $\langle Q^4\rangle_c = \langle Q^4\rangle - 3\langle Q^2\rangle^2$.

Like in the case of the topological susceptibility, also the definition of $\langle Q^4\rangle$ needs a special prescription for the contact terms, in order to correspond to the quantity which enters the Taylor expansion of $F(\theta)$. Starting from the lattice definition, Q_L, one can define the expectation value

$$\langle Q_L^4\rangle = \int \mathrm{d}^4x_1 \ldots \mathrm{d}^4x_4 \langle q_L(x_1)q_L(x_2)q_L(x_3)q_L(x_4)\rangle \tag{2.13}$$

and it is clear that, apart from an obvious multiplicative renormalization constant $Z^4(\beta)$, $\langle Q_L^4\rangle$ will be linked to $\langle Q^4\rangle$ by additive renormalizations related to the contact terms arising when two or more charge densities in the expectation value integrated in Eq. (2.13) come to the same point. Our aim is to eventually compute the renormalization constants numerically, and in this sense we are not interested in the exact form of the mixing terms, but just in understanding if they can be related in a simple way to the correlation functions of different order, $\langle Q^m\rangle$, so that they can be computed using the heating method, as it will be clarified below.

We will assume a simple and quite natural form for the renormalization rule:

$$\langle Q_L^4\rangle \;=\; Z(\beta)^4\langle Q^4\rangle + M_{4,2}(\beta)\langle Q^2\rangle + M_{4,0}(\beta)\ , \tag{2.14}$$

where $M_{4,2}(\beta)$ and $M_{4,0}(\beta)$ are two constants which are independent of the topological sector. We will discuss in the following whether Eq. (2.14) makes sense from a theoretical point of view, while its validity will be fully checked numerically in Section 3.

The presence of the term $Z(\beta)^4\langle Q^4\rangle$ in Eq. (2.14) comes from the multiplicative renormalization of the topological charge density. The question is then whether the additive renormalizations coming from contact terms can be put in the form $M_{4,2}(\beta)\langle Q^2\rangle+M_{4,0}(\beta)$. Contact terms arise when two or more charge densities in the expectation value in Eq. (2.13) come to the same point, but the discussion of the two charge case will suffice: the instance with three (or more) charge densities coming to the same point can be considered as a special case of the two charge case, so that the related mixing terms are already considered when discussing the two charge contact term.

Let us consider for instance $x_3 \sim x_4$ in Eq. (2.13). The operators of lower dimension appearing in the OPE of $q_L(x_3)q_L(x_4)$ are the identity operator and the action density $s(x) \propto F^a_{\mu\nu}(x)F^a_{\mu\nu}(x)$. The insertion of the identity operator in the expectation value in Eq. (2.13) leads to a contribution proportional to

$$\int \mathrm{d}^4x_1\mathrm{d}^4x_2\ \langle q_L(x_1)q_L(x_2)\ \mathrm{Id}\rangle = \langle Q_L^2\rangle = Z^2(\beta)\langle Q^2\rangle + V\ M(\beta)\ , \tag{2.15}$$

which is consistent with the assumption in Eq. (2.14). The insertion of the action density operator leads to a contribution proportional to

$$\int \mathrm{d}^4x_1\mathrm{d}^4x_2\mathrm{d}^4x\langle q_L(x_1)q_L(x_2)s(x)\rangle = \langle Q_L^2 S\rangle = \langle S\rangle\langle Q_L^2\rangle - \frac{d}{d\beta}\langle Q_L^2\rangle\ , \tag{2.16}$$

where S is the total action of the theory and we have used the relation, which is valid for any operator O, $(d/d\beta)\langle O\rangle = \langle S\rangle\langle O\rangle - \langle SO\rangle$, where the derivative is taken as the four dimensional volume in lattice units, V, is kept fixed. The first term on the right hand side of Eq. (2.16), $\langle S\rangle\langle Q_L^2\rangle$, is proportional to $Z^2(\beta)\langle Q^2\rangle + V\ M(\beta)$ and therefore consistent with Eq. (2.14). Using the fact that the topological susceptibility χ is a renormalization group invariant quantity, i.e. independent of β, and that $\chi = \langle Q^2\rangle/(Va^4)$, the second term can be written as

$$
\begin{aligned}
\frac{d}{d\beta}\langle Q_L^2\rangle &= \frac{d}{d\beta}\big(Z^2(\beta)\chi a^4(\beta)V + M(\beta)V\big) = \chi V\frac{d}{d\beta}(Z^2(\beta)a^4(\beta)) + V\frac{dM(\beta)}{d\beta} = \\
&= \langle Q^2\rangle a^{-4}(\beta)\frac{d}{d\beta}(Z^2(\beta)a^4(\beta)) + V\frac{dM(\beta)}{d\beta}\ , \qquad (2.17)
\end{aligned}
$$

which is again consistent with Eq. (2.14).

This does not complete the discussion, as operators of higher dimension in the OPE of $q_L(x_3)q_L(x_4)$ could bring corrections in which cannot be expressed in the same simple form as in Eq. (2.14). However we will assume those corrections to be negligible, and this assumption will be well supported by the numerical data shown in Section 3.

In order to extract the value of $\langle Q^4\rangle$ from Eq. (2.14), we need to measure the lattice expectation value $\langle Q_L^4\rangle$, to already know $\langle Q^2\rangle$, and to determine the new renormalization constants $M_{4,2}(\beta)$ and $M_{4,0}(\beta)$. The computation of the renormalization constants can be performed using a simple extension of the heating method. Indeed, measuring the expectation value $\langle Q_L^4\rangle$ on the ensemble thermalized around a semi-classical configuration of charge Q, one obtains

$$\langle Q_L^4\rangle = Z^4(\beta)\ Q^4 + M_{4,2}(\beta)\ Q^2 + M_{4,0}(\beta)\ . \qquad (2.18)$$

It is clear that if we repeat the measurement in 2 sectors with different values of Q (for instance $Q = 0, 1$), we obtain 2 different constraints involving the renormalization constants which, assuming that $Z(\beta)$ is already known, allow the determination of $M_{4,2}(\beta)$ and $M_{4,0}(\beta)$. If we perform the measurement in more than 2 sectors we have more constraints than constants to be determined, and this offers the possibility to perform a non-trivial test of Eq. (2.14) and of the heating method.

We close this Section by considering the general case of the n-th order correlation function. A natural extension of Eq. (2.14) is the following:

$$\langle Q_L^n\rangle = Z(\beta)^n\langle Q^n\rangle + \sum_{h=1}^{n/2} M_{n,n-2h}(\beta)\langle Q^{n-2h}\rangle\ , \qquad (2.19)$$

and its validity can be discussed along the same lines as for $n = 4$. In this case, the measurement of $\langle Q_L^n\rangle$ on the ensemble thermalized around a semi-classical configuration of charge Q gives

$$\langle Q_L^n \rangle = Z^n Q^n + M_{n,n-2} Q^{n-2} + \ldots + M_{n,0} \ , \tag{2.20}$$

so that it is necessary to measure $\langle Q_L^n \rangle$ in at least $n/2$ different topological sectors to determine the $n/2$ renormalization constants $M_{n,n-2}(\beta), M_{n,n-4}(\beta), \ \ldots \ , M_{n,0}(\beta)$.

3. Determination of $\langle Q^4 \rangle_c$ in $SU(3)$ pure gauge theory

In this Section we present numerical results obtained for $SU(3)$ pure gauge theory. We will illustrate a detailed study of the renormalization constants involved in the determination of $\langle Q^2 \rangle$ and $\langle Q^4 \rangle$, using the heating method: we will employ samples of configurations thermalized in three different topological sectors, $Q = 0, 1, 2$, and this will enable us to perform a non-trivial consistency test of Eq. (2.14) and of the heating method itself. We will then combine the values of the renormalization constants with the results obtained at equilibrium to compute $\langle Q^4 \rangle_c$ and thus obtain information about the quartic term in the expansion of $F(\theta)$. In particular we will compute the quantity $b_2 = -\frac{\langle Q^4 \rangle_c}{12 \langle Q^2 \rangle}$, which measures the relative weight of quartic to quadratic terms and has been determined in Ref. [7] via the cooling method*.

All the results reported in this Section refer to simulations performed on a lattice of size 16^4, with $\beta = 6.1$ and the standard Wilson action. Two different discretized topological charge density operators have been used, corresponding to the 1-smeared and 2-smeared operators defined in Section 2.

3.1. Determination of the renormalization constants

We will make use of the method described in Section 2 to determine the renormalization constants which enters the computation of $\langle Q^2 \rangle$ and $\langle Q^4 \rangle$.

We have collected five different samples of configurations, one thermalized in the $Q = 0$ sector (around the zero field configuration), two in the $Q = 1$ sector (thermalized around two different semiclassical configurations of topological charge one) and two in the $Q = 2$ sector (thermalized around two different semiclassical configurations of topological charge

*We use the same notation used in Ref. [7], in order to make the comparison easier.

two). The semiclassical configurations have been obtained by extracting thermalized configurations with non-trivial topology from the equilibrium ensemble at $\beta = 6.1$ and then minimizing their action by a usual cooling technique. All the five samples have been obtained by performing about 3000 heating trajectories around the semiclassical configurations, each trajectory consisting of 90 heating steps; 6 straight cooling steps have been applied on heated configurations to check that their background topological content did not change.

We have then measured the expectation values $\langle Q_L^2 \rangle$, $\langle Q_L^4 \rangle$, and also $\langle Q_L \rangle / Q$ where $Q \neq 0$, over the five samples, with the aim of applying Eqs. (2.8), (2.9), (2.18) and determine the renormalization constants†. We have reported the results in Table I for the 1-smeared operator and in Table II for the 2-smeared operator: expectation values obtained on samples with the same Q turned out to be equal within errors, as they should, and we have reported in the tables only their weighted averages. It is still possible to appreciate in Table I and II the agreement for the values of Z determined in the $Q = 1$ and $Q = 2$ sectors. We have also reported results for $\langle Q_L^6 \rangle$, which will be used in Section 4.

Let us rewrite Eq. (2.7) in the form $\langle Q_L^2 \rangle = Z(\beta)^2 \langle Q^2 \rangle + M_{2,0}(\beta)$, with $M_{2,0}(\beta) = VM(\beta)$. The information contained in $\langle Q_L^2 \rangle$ for each different topological sector Q can be used to determine $M_{2,0}$, using Eq. (2.9). We have 2 constants to be determined, Z and $M_{2,0}$, and 3 equations ($Q = 0, 1, 2$), plus two direct determinations of Z from $\langle Q_L \rangle / Q$, so that there are 5 constraints to be satisfied and only 2 variables to be determined. The fact that this can be done consistently is a non-trivial test of the method, and more precisely of the fact that the UV fluctuations which are responsible for the renormalization constants are decoupled from the background topological content, an assumption that is at the very basis of the heating method, as it has been explained in Section 2. In practice we have used the 5 values measured for $\langle Q_L^2 \rangle$ and $\langle Q_L \rangle / Q$ to perform a best fit to Eqs. (2.8) and (2.9), obtaining best fit values which are reported in Table III and good χ^2/d.o.f. values (~ 0.1 for the 1-smeared operator and ~ 0.2 for the 2-smeared operator‡). The values

†The initial charge of the semiclassical configuration used in the heating procedure, Q, is never strictly an integer (apart from the case $Q = 0$). The deviation from the corresponding integer value is always around 3% in our case (e.g., when $Q \sim 1$, we actually have $Q \simeq 0.97$). When applying Eqs. (2.8), (2.9) and (2.18), one has to be careful and make use of the real value of Q instead of the closest integer. For a more accurate discussion on this point see for instance Ref. [20].

‡The low values obtained for χ^2/d.o.f. can be related to the fact that the measurements of $\langle Q_L^2 \rangle$ and $\langle Q_L \rangle / Q$ at corresponding values of Q are partially correlated, since they are measured on the same sample of configurations.

obtained for Z and $M_{2,0}$ are compatible with those reported in Ref. [14].

The same procedure has been repeated, using the $\langle Q_L^4 \rangle$ measurements and Eq. (2.18), to obtain the best fit values for $M_{4,2}$ and $M_{4,0}$ reported in Table III. Also in this case we have obtained good values for χ^2/d.o.f. (~ 0.1 for both the 1-smeared and the 2-smeared operator). This represents a strong numerical support to the validity of Eq. (2.14).

3.2. Determination of $\langle Q^2 \rangle$, $\langle Q^4 \rangle$, and $\langle Q^4 \rangle_c$

Now that we have determined the renormalization constants we can proceed to determine $\langle Q^2 \rangle$ and $\langle Q^4 \rangle$. The equilibrium values for $\langle Q_L^2 \rangle$ and $\langle Q_L^4 \rangle$, which are reported in Table IV, have been measured on a sample of 300K configurations separated by five updating cycles, each composed of a mixture of 4 over-relaxation + 1 heat-bath updating sweeps; the reported errors have been estimated by a standard blocking technique.

The value of $\langle Q^2 \rangle$ can be computed as

$$\langle Q^2 \rangle = \frac{\langle Q_L^2 \rangle - M_{2,0}}{Z^2} \ . \tag{3.1}$$

The expression for $\langle Q^4 \rangle$ follows from Eq. (2.14):

$$\langle Q^4 \rangle = \frac{\langle Q_L^4 \rangle - M_{4,2} \langle Q^2 \rangle - M_{4,0}}{Z^4} \ . \tag{3.2}$$

The results for $\langle Q^2 \rangle$ and $\langle Q^4 \rangle$ are reported in Table IV, the errors have been computed by standard error propagation. It is interesting to notice that the values obtained for the 1-smeared operator and for the 2-smeared operator are in good agreement, as they should, again confirming the robustness of the method. We can finally determine $\langle Q^4 \rangle_c = \langle Q^4 \rangle - 3\langle Q^2 \rangle^2$, obtaining $\langle Q^4 \rangle_c = 0.32 \pm 1.80$ for the 1-smeared and $\langle Q^4 \rangle_c = 0.66 \pm 0.90$ for the 2-smeared operator, leading to $b_2 = -0.012(62)$ and $b_2 = -0.024(32)$ for the 1-smeared and 2-smeared operator respectively, in agreement with the determination reported in Ref. [7].

4. A closer look into the renormalization effects

The renormalization constants Z, $M_{n,m}$ ($m < n$) which, for a given lattice discretization Q_L, appear in Eq. (2.19), are in principle independent of each other, or at least no simple relation exists among them, unless some further hypothesis can be done about the nature of the UV fluctuations which are responsible for the renormalizations. In this Section we will propose and test an ansatz which will greatly simplify the structure of the renormalization constants and will lead to a renormalization formula which directly involves the connected correlation functions, thus allowing a more precise determination of b_2.

An hypothesis about the nature of the UV fluctuations has been done in Refs. [9, 11], where it was assumed that the discretized topological charge density can be expressed as

$$q_L(x) \simeq [Z + \zeta(x)]q(x) + \eta(x) , \tag{4.1}$$

where $q(x)$ is a background topological charge density which is determined by physical fluctuations on the scale of the correlation length ξ, whereas $\zeta(x)$ and $\eta(x)$ are random variables with zero averages which are determined by the short range UV fluctuations and, at least in the continuum limit, are expected to be decoupled from $q(x)$, i.e. $\langle\zeta(x)q(x)\rangle = \langle\eta(x)q(x)\rangle = 0$. Summing Eq. (4.1) over all lattice points, the following relation follows for the lattice topological charge Q_L:

$$Q_L = Z\, Q + \sum_x \zeta(x)q(x) + \eta , \tag{4.2}$$

where $\eta = \sum_x \eta(x)$. We now make the further assumption that the term $\sum_x \zeta(x)q(x)$ in Eq. (4.2) can be neglected, configuration by configuration. This is not unreasonable, in view of the fact that $q(x)$ and $\zeta(x)$ are decoupled from each other. We will thus assume that

$$Q_L = Z\, Q + \eta , \tag{4.3}$$

where η is a random noise with zero average which is stochastically independent of Q.

This assumption has relevant consequences for the structure of the renormalization constants. Indeed, using the hypothesis that Q and η are stochastically independent variables and that they are both evenly distributed around zero, it is easy to verify that the general renormalization formula in Eq. (2.19) becomes

$$\langle Q_L^n\rangle = \sum_{h=0}^{n/2} \binom{n}{2h} Z^{n-2h}\langle Q^{n-2h}\rangle\langle\eta^{2h}\rangle , \tag{4.4}$$

so that the renormalization relation for $\langle Q_L^n\rangle$ is described only in terms of Z and of the correlation functions of the noise η. In particular we have $M_{n,m} = \binom{n}{m} Z^m\langle\eta^{n-m}\rangle$, a relation that should be verified on numerical data if our ansatz in Eq. (4.3) is correct. From the data in Table III it can be checked that indeed $M_{4,2} = 6Z^2\langle\eta^2\rangle = 6Z^2 M_{2,0}$, but we will now proceed further and check the validity of Eq. (4.4) up to $n = 6$. The correlation functions of η can be determined by the heating method using the analogous of Eq. (2.20), which up to $n = 6$ reads:

$$\begin{aligned}
\langle Q_L^2\rangle &= Z^2Q^2 + \langle\eta^2\rangle \\
\langle Q_L^4\rangle &= Z^4Q^4 + 6Z^2Q^2\langle\eta^2\rangle + \langle\eta^4\rangle \\
\langle Q_L^6\rangle &= Z^6Q^6 + 15Z^4Q^4\langle\eta^2\rangle + 15Z^2Q^2\langle\eta^4\rangle + \langle\eta^6\rangle \ .
\end{aligned} \tag{4.5}$$

Using the values for $\langle Q_L^2\rangle$, $\langle Q_L^4\rangle$ and $\langle Q_L^6\rangle$ obtained in the sectors with $Q = 0, 1, 2$ and reported in Tables I and II, we have performed a best fit to Eqs. (4.5), obtaining the best fit values reported in Table V with $\chi^2/\mathrm{d.o.f.} \simeq 0.34$ for the 1-smeared operator and $\chi^2/\mathrm{d.o.f.} \simeq 0.23$ for 2-smeared operator. The fact that the values for $\langle Q_L^2\rangle$, $\langle Q_L^4\rangle$ and $\langle Q_L^6\rangle$ obtained in the various sectors can be fitted by the simple relations in Eq. (4.5) is a confirmation of the validity of the ansatz in Eq. (4.3).

Assuming that Eq. (4.3) is valid, it is possible to write a renormalization relation which involves directly the connected correlation functions. Indeed, it is a general rule that the connected correlation functions of a stochastic variable (Q_L in our case), which is the sum of two variables which are stochastically independent of each other (ZQ and η in our case), are the sum of the corresponding connected correlation functions, i.e.

$$\langle Q_L^n\rangle_c = Z^n\langle Q^n\rangle_c + \langle\eta^n\rangle_c \ . \tag{4.6}$$

Therefore in order to compute $\langle Q^n\rangle_c$ we need to know, apart from Z, only one renormalization constant, $\langle\eta^n\rangle_c$, which can be easily measured by computing $\langle Q_L^n\rangle_c$ on the sample of configurations in the $Q = 0$ sector. $\langle Q^n\rangle_c$ is then given by

$$\langle Q^n\rangle_c = \frac{\langle Q_L^n\rangle_c - \langle\eta^n\rangle_c}{Z^n} \ , \tag{4.7}$$

where $\langle Q_L^n\rangle_c$ is measured on the ensemble of configurations at equilibrium.

We have computed $\langle Q_L^4\rangle_c = \langle Q_L^4\rangle - 3\langle Q_L^2\rangle^2$ on our equilibrium configurations at $\beta = 6.1$, obtaining $\langle Q_L^4\rangle_c = 0.026(7)$ for the 1-smeared operator and $\langle Q_L^4\rangle_c = 0.057(13)$ for the 2-smeared operator. We have then computed $\langle Q_L^4\rangle_c$ on our sample of configurations thermalized in the $Q = 0$ sector at $\beta = 6.1$, obtaining $\langle\eta^4\rangle_c = \langle\eta^4\rangle - 3\langle\eta^2\rangle^2 = 0.006(4)$ for the 1-smeared operator and $\langle\eta^4\rangle_c = 0.001(2)$ for the 2-smeared operator. In both cases (equilibrium and $Q = 0$) errors have been estimated by standard jackknife techniques.

By using Eq. (4.7) and the values for Z and $\langle Q^2 \rangle$ previously obtained, we have obtained $\langle Q^4 \rangle_c = 0.68(24)$, $b_2 = -0.024(9)$ for the 1-smeared operator and $\langle Q^4 \rangle_c = 0.66(15)$, $b_2 = -0.024(6)$ for the 2-smeared operator.

By making use of the ansatz in Eq. (4.3) we have thus made determinations which are much more precise than those obtained in Section 3. The reason is that Eq. (4.6) allows to relate $\langle Q^n \rangle_c$ directly to the connected correlation functions of the discretized lattice topological charge, with only two renormalization constants involved: this greatly simplifies computations and error propagation, thus leading to improved estimates. We notice that most of the error in the final determination of $\langle Q^4 \rangle_c$ and b_2 comes from the determination of $\langle Q_L^4 \rangle_c$ at equilibrium, which is also the most expensive part of the computation in terms of CPU time. The renormalization procedure is thus completely under control and numerically non expensive.

We have also made a determination of b_2 at $\beta = 6.0$, again on a 16^4 lattice. On a sample of about 300K configurations obtained at equilibrium and using the same algorithm as for $\beta = 6.1$ we have obtained, for the 2-smeared operator, $\langle Q_L^2 \rangle = 1.377(7)$, $\langle Q_L^4 \rangle_c = 0.052(23)$. On a sample of configurations thermalized in the $Q = 0$ topological sector by performing about 3000 heating trajectories, each composed of 90 heating steps, we have obtained, for the 2-smeared operator, $\langle \eta^2 \rangle = 0.308(10)$ and $\langle \eta^4 \rangle_c = 0.002(3)$. From these data, using the value $Z(\beta = 6.0) = 0.51(2)$ reported for the 2-smeared operator in Ref. [14], we obtain $b_2 = -0.015(8)$, which is consistent with the value obtained at $\beta = 6.1$.

Let us close this Section with some further speculations about the nature of the UV fluctuations. The value obtained for $\langle \eta^4 \rangle_c$ is very small and compatible with zero for both the 1-smeared and the 2-smeared operator. We have also measured $\langle \eta^6 \rangle_c$ on the sample of configurations at $Q = 0$ obtaining $\langle \eta^6 \rangle_c = 0.001(8)$ for the 1-smeared and $\langle \eta^6 \rangle_c = 0.0005(14)$ for 2-smeared operator ($\beta = 6.1$). This seems to indicate that η behaves as a Gaussian noise: it can also be verified on the values reported in Table V that $\langle \eta^4 \rangle$ is always compatible with $3\langle \eta^2 \rangle^2$ and that $\langle \eta^6 \rangle$ is always compatible with $15\langle \eta^2 \rangle^3$, as it should be for a Gaussian variable. We have also directly verified on the histograms of the distribution of η in the $Q = 0$ sector that it does not present any significant deviation from a Gaussian distribution. If the hypothesis of Gaussian distribution for η were true, the renormalization relation in Eq. (4.6) would become, for $n > 2$, $\langle Q_L^n \rangle_c = Z^n \langle Q^n \rangle_c$, i.e. the connected correlation functions of Q_L would renormalize only multiplicatively for $n > 2$. However we will not consider further analysis of this hypothesis in the present paper.

5. Conclusions

In this paper we have discussed how to extend the field theoretical method, already used for the lattice determination of the topological susceptibility, in order to compute further terms in the expansion of the ground state energy $F(\theta)$ around $\theta = 0$.

After a review of the method as used for the determination of the topological susceptibility, we have discussed the structure of the renormalizations involved in the general case and how they can be computed using the heating method. We have presented numerical results regarding $SU(3)$ pure gauge theory, providing both support to the correctness of the method and a determination of the fourth order term in the expansion of $F(\theta)$ around $\theta = 0$.

In the last part of the paper we have made some speculations about the nature of the lattice UV fluctuations which are responsible for the renormalizations and proposed an ansatz, which we have verified against the numerical data, that leads to a simpler structure for the renormalizations and to an improved estimate of the fourth order term.

The determinations obtained are in agreement with those obtained in Ref. [7] via the cooling method, and confirm that fourth order corrections to the simple θ^2 behaviour of $F(\theta)$ around $\theta = 0$ are small already for $N = 3$.

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TABLE CAPTIONS

Tab. I. Expectation values measured in different topological sectors for the 1-smeared operator.

Tab. II. Expectation values measured in different topological sectors for the 2-smeared operator.

Tab. III. Values of the renormalization constants obtained by using the results reported in Tables I and II and performing a best fit to Eqs. (2.8), (2.9) and (2.18).

Tab. IV. Expectation values measured at eequilibrium and results obtained for the renormalized quantities.

Tab. V. Values of the renormalization constants obtained by using the results reported in Tables I and II and performing a best fit to Eqs. (2.8) and (4.5).

Table I

Q	$Z = \langle Q_L \rangle / Q$	$\langle Q_L^2 \rangle$	$\langle Q_L^4 \rangle$	$\langle Q_L^6 \rangle$
0	–	0.311(12)	0.290(20)	0.48(5)
1	0.416(6)	0.4785(60)	0.630(15)	1.295(45)
2	0.413(5)	0.9626(80)	1.973(50)	5.82(18)

Table II

Q	$Z = \langle Q_L \rangle / Q$	$\langle Q_L^2 \rangle$	$\langle Q_L^4 \rangle$	$\langle Q_L^6 \rangle$
0	–	0.208(10)	0.124(10)	0.131(18)
1	0.544(5)	0.489(5)	0.556(12)	0.93(3)
2	0.542(4)	1.314(8)	2.77(6)	7.65(17)

Table III

operator	Z	$M_{2,0}$	$M_{4,2}$	$M_{4,0}$
1 − smeared	0.414(4)	0.315(6)	0.336(16)	0.289(16)
2 − smeared	0.543(5)	0.211(5)	0.377(15)	0.124(9)

Table IV

operator	$\langle Q_L^2 \rangle$	$\langle Q_L^4 \rangle$	$\langle Q^2 \rangle$	$\langle Q^4 \rangle$
1 − smeared	0.7121(38)	1.548(18)	2.312(72)	16.4 ± 1.8
2 − smeared	0.8776(60)	2.368(36)	2.262(41)	16.02(72)

Table V

operator	Z	$\langle \eta^2 \rangle$	$\langle \eta^4 \rangle$	$\langle \eta^6 \rangle$
1 − smeared	0.415(4)	0.315(6)	0.298(11)	0.462(37)
2 − smeared	0.542(4)	0.211(5)	0.129(6)	0.131(17)